

TIR a cup of tea, and watch how the tea leaves swirl and dip. Imagine what it might take to predict that movement, given only the initial forces and conditions of cup, tea, spoon, and leaves. Now add milk. The more-or-less orderly motion of tea and leaves suddenly becomes incredibly more complex, as do the forces that drive the flow and eddies of the liquids. The pathway to understanding and prediction becomes less clear as well. Welcome to the world of fluid dynamics—the study of fluids in motion.

Lawrence Livermore physicists Paul Miller and Andrew Cook delved into the details of fluids on the move to simulate an experiment conducted at the University of Arizona (UA) and predict interactions of two dissimilar liquids. With the help of powerful visualization tools created by Livermore computer scientist Peter Lindstrom, they revealed the inner workings of a perplexing characteristic that, under certain situations, is key to the mixing of dissimilar fluids. Termed centrifugal baroclinic instability, the phenomenon embodies the interaction of two fluids with varying pressures and densities as they spin around each other. This fluid dynamic dance occurs in a broad range of circumstances, from deep ocean eddies to convection currents in the cores of dying stars.

Doing the Bounce

Miller and Cook's work had its genesis with a UA experiment to explore what happens at the interface between

two liquids of different densities when that interface is

In the experiment, conducted by UA professor Jeffrey Jacobs and former UA graduate student Charles Niederhaus (now with the National Aeronautics and Space Administration), a small rectangular transparent tank was mounted on vertical rails and suspended above a spring on a platform. The tank contained a heavier liquid (salt water) and a lighter liquid (an alcohol—water mix). Initially, it was moved from side to side to set up standing waves on the liquid interface. Then the tank was released, falling and bouncing off the spring before coasting up and down to a final stop. Since the tank was essentially in free-fall before and after the bounce, the only force the liquids experienced was the sharp acceleration—50 times that of gravity—of the 30-millisecond bounce. A video camera documented what happened at the liquid interface from initial standing wave to the final jolt.

The part of the experiment that interested Miller and Cook was the 1 second after the bounce during which the tank is again in free-fall. At bounce time, the acceleration pushed the peak of the standing wave down, while the trough moved upward. These opposing actions resulted from a twisting force (a torque) acting on the liquid interface. In this case, the twisting is called baroclinic torque because it involves

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differing pressures (baro) and inclined (clinic) density interfaces. In stable configurations—when light fluid is on top of heavy fluid, for instance—baroclinic torque drives phenomena such as ocean waves. In unstable configurations—when heavy fluids are on top of light or when fluids in a stable configuration are accelerated—baroclinic torque drives Rayleigh—Taylor and Richtmyer—Meshkov instabilities. These instabilities typically lead to mushroom-shaped structures forming in fluids. In the UA experiment, the fluids continued to move after the bounce, forming these mushroom shapes, with the interface rolling up at the sides of the mushroom.

What happened at the core of this roll-up drew Miller and Cook's attention. Rather than a smooth, continual spiral inward, the roll-up began to disintegrate because of a small secondary instability. (The primary instability was the Richtmyer–Meshkov instability that created the large-scale roll-up.) "This secondary instability happens long after the bounce," explains Miller, "so it was not caused by the acceleration of the bounce itself. The source of these perturbations deep inside the vortex and how they evolved were not well understood."

Turning and Turning in the Widening Gyre

To gain insights into the nature of these secondary instabilities, Miller and Cook used MIRANDA, a direct numerical simulation code created by Cook. MIRANDA's hybrid spectral and compact-finite-difference algorithms resolve all scales of motion in a flow, down to the viscous and diffusive scales. "These were direct numerical simulations, meaning we tried to work from first principles—or as close as we could get—without making assumptions or using models for some of the smaller dynamics of the system," says Miller.

The computational mesh was a two-dimensional slab one cell thick (1,025 by 1 by 5,000 grid points). Each computational cell was 41 micrometers across, or less than half the width of a human hair. "Since the experiment was essentially two dimensional," says Miller, "we were able to increase the resolution by running a two-dimensional simulation. Particularly in the timeframe we were interested in, three-dimensional physics—such as three-dimensional tilt or stretch in the vortices—doesn't play an important role."

The simulation ran on 64 of the 1,088 processors that make up ASCI Frost, the unclassified portion of the Advanced Simulation and Computing (ASCI) Program's White supercomputer system. The simulation re-creates 2.5 seconds from the experiment, starting with the motion of the initial standing wave and continuing for about 1 second after the

bounce. Re-creating the details of the wave allowed Miller and Cook to replicate the low-level velocity from the wave that was present when the bounce occurred.

The results of that calculation were then used to simulate the instabilities that developed during and after the bounce,

Flying through the Data

Once Livermore physicists Paul Miller and Andrew Cook ran their simulation, they were faced with the need to interpret their results, so they turned to computer scientist Peter Lindstrom for help in visualizing their data. Lindstrom explains that he specializes in creating tools to visualize giant data sets. One of these is a software tool called Visualization Streams for Ultimate Scalability (ViSUS). Lindstrom worked closely with Miller and Cook to create movies that looked at how quantities such as density and pressure varied over time and space and how they correlated with the vorticity—that is, how much local rotation was generated in the fluid, in what areas, and in what direction. Some of the visualizations incorporate as many as five variables: two spatial dimensions, vorticity, vorticity production, and time.

"We also worked up a tool that allows researchers to interact with a 3D simulation," Lindstrom explains. "Basically, we put them in the driver's seat, giving them full control over the visualization parameters so they can explore and interact with their data in ways that are useful to them. This is potentially so much more powerful than having someone such as me create a single image or canned movie where all the parameters are fixed. It is not likely that a single setting of many parameters is sufficient or that I know exactly what to emphasize in the visualization. Also, for large data sets-and in particular threedimensional data where things might be occluded or hidden deep within the data—the scientist needs to be able to move around the data set to obtain the most meaningful picture of the data. With ViSUS, the scientist can zoom in on small features, look at more global trends in the data, and explore it from many different vantage points, while at the same time turning the control knobs for the visualization itself. This control is possible only with interactive visualization."

Such tools allow researchers to look at the simulation while it is progressing, so they can stop it—to tinker with the mesh, for instance—and correct it as needed. No longer do they need to wait two weeks for a visual result to make corrections. Tools such as ViSUS are beginning to show up on physicists' desktops and will, in the long run, only make it easier for scientists to stay on top of complex simulations created on the Advanced Simulation and Computing Program's supercomputing systems.

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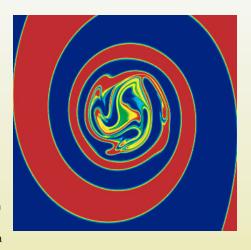
About the Simulations

The high-fidelity computer simulations developed by Livermore's Andrew Cook and Paul Miller were carried out on a 1,025- by 5,000- node mesh, at a Schmidt number of 100, and a circulation Reynolds number of 3,800. A suite of two-dimensional animations of calculated quantities and a fly-over of a three-dimensional animated rendering of the vorticity field

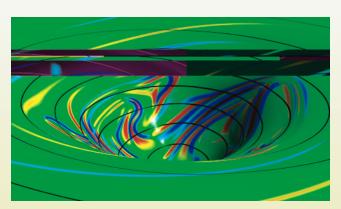
allowed researchers to visualize the fluid flow as it developed. All of the still shots below were taken at the same time (0.75 second after the bounce). The award-winning movie "Visualizations of the Dynamics of a Vortical Flow" is available online at the VIEWS Visualization Project: Image and Movie Gallery www.llnl.gov/icc/sdd/img/images.shtml.

Fluid density visualization. Red shows the higher density liquid and blue the lower. Green shows where the two liquids have mixed. The interface between the two liquids is rolled up around a

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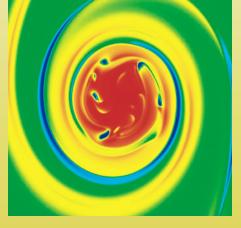
large vortex in the middle. In the core of the vortex, where a low-pressure region exists, the secondary instability has led to increased mixing of the two fluids.



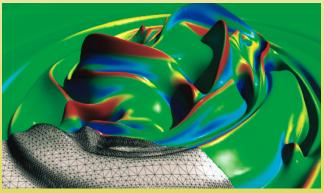
Pressure (shown by height and contour lines) visualization with a superimposed color map of the vorticity production (or baroclinic torque). Areas of fluid rotation are springing up on the sides of the pressure well where the change in pressure is steepest. Clockwise and counterclockwise vortices are generated in alternating thin sheets. Eventually, these small areas of oppositely rotating fluid will break down the orderly structure of the rolled-up fluids, resulting in increased mixing.

Vorticity (local fluid rotation) visualization. Red and its variants (yellow and orange) indicate areas where liquid is rotating in a counterclockwise direction; blue indicates areas

where it is rotating



in a clockwise direction. Green represents areas where no rotation is taking place. The pockets and strips of blue in the midst of the red core indicate areas that have been affected by the secondary instability and are rotating in the opposite direction from the surrounding fluid.

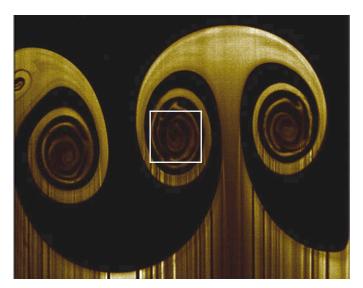


Vorticity production visualized onto a heightmap of the vorticity field, with the visualization mesh partially exposed. Peaks are areas of most counterclockwise rotation; valleys are areas of highest clockwise rotation. Flat surrounding areas are locations of little or no rotation. The colors show vorticity being produced by the secondary instability. Red indicates counterclockwise rotation; blue indicates clockwise rotation. Blue patches on high peaks are particularly telling. Since the rotation being produced (clockwise) does not correlate with the rotation that is ongoing (counterclockwise), the secondary instability is responsible.

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particularly the secondary instability in the core of the vortex. By using visualization software developed by Peter Lindstrom of the Center for Applied Scientific Computing (see the box on p. 23), Miller and Cook discovered the cause of this secondary instability—the interaction of the low-pressure field in the center of the vortex (similar to the low-pressure "eye" in the center of a cyclone or the "well" that appears in the cup of vigorously stirred tea) with the varying densities in the fluid whirling around in the vortex.

According to Miller, this instability evolves as follows. The interface of the two liquids begins to roll up because of the vorticity deposited by the bounce. The simulation (see the box on p. 24) shows that at the start of this process, the two liquids remain mostly unmixed, curling around the center of the roll-up and forming a spiral pattern. As the liquid interface spirals inward, centrifugal force (the pseudoforce that appears to push matter outward from the center of rotation) comes into play, producing a low-pressure well at the center of the evolving "jelly roll." The pressure increases up the sides of this well, while the density alternates between light and heavy. Prior to the secondary instability, all of the fluid spins counterclockwise. The interaction of varying pressure and density generates new vortices-some spinning clockwise, others counterclockwise—on the sides of the pressure well. These tiny harbingers of disorder increase in number, spread,



One image from a set taken during a University of Arizona experiment exploring the interface between two liquids—one of lighter density (black) and one of heavier density (white)—when the interface was accelerated. This image was taken 749 milliseconds after acceleration. Livermore physicists wanted to uncover the mechanism that destroyed the orderly roll-up in the sides of the mushroom shape (boxed in white).

and grow, eventually leading to the breakdown of the orderly spiral of fluids and an increase in fluid mix.

The visualizations created by Lindstrom allowed Miller and Cook to more easily see correlations and relationships in their numerical results, which included data on pressure, density, vorticity, and vorticity production (baroclinic torque) at different points in time during the experiment.

From Fusion Pellets to Planet Rotation

Cook and Miller validated their simulations using data from the UA experiment and presented the results of their research at the 55th Annual Meeting of the American Physical Society, Division of Fluid Dynamics, held in Dallas, Texas, in November 2002. A video created with Lindstrom describing their work and highlighting the visualizations was honored in the meeting's "Gallery of Fluid Motion."

Understanding such fluid instabilities—how and why they form and evolve and being able to predict them—is important to understanding how fluids, including both liquids and gases, behave. Such instabilities occur on scales from the microscopic to astronomical and can have a dramatic effect. Richtmyer—Meshkov instabilities, for instance, may affect the performance of laser fusion pellets and nuclear weapons and can occur in the explosions of supernovas. "After all," Miller concludes, "the same physical laws that apply to supernovas govern a cup of tea."

-Ann Parker

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Key Words: centrifugal baroclinic torque, fluid dynamics, Richtmyer–Meshkov instability, secondary instability.

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To view a video of the University of Arizona experiment, see: info-center.ccit.arizona.edu/~fluidlab/incomp.html

To view the "Visualizations of the Dynamics of a Vortical Flow," the award-winning video on the work described in this article, see: www.llnl.gov/icc/sdd/img/images/aps02.mov

To view examples from the American Physical Society's "Gallery of Fluid Motion," see:

ojps.aip.org/phf/gallery/index1.jsp

[The work discussed in this article is scheduled to be posted to the APS site during 2003.]